

# NUMERICAL SIMULATION FOR DROPLET COMBUSTION USING LAGRANGIAN HYDRODYNAMICS

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A predictive model of spray combustion must incorporate models for the wide variety of physical environments in a practical combustor. In regions where droplets are closely spaced, combustion resembles a diffusion flame; where they are well-separated, an envelope or wake flame results. The relative velocity field between the fuel droplets and oxidizer influences boundary layer development about the droplet, recirculating flow patterns, and droplet shape and stability. A model must encompass these interacting temporal and spatial effects as well as complicated combustor boundaries. The objective of the current work is to develop the triangular gridding method for describing the individual and collective properties of vaporizing and burning fuel droplets.

Our approach to this problem has been to modify the basic two dimensional Lagrangian model [1] to simulate flows in and about fuel droplets [2]. This general-connectivity triangular grid permits accurate representation of boundaries as well as material surfaces and interfaces. It also allows variable resolution through the insertion of new cells as required to maintain accuracy. The finite-difference operators for divergence, curl and gradient are constructed to exactly reflect the properties of the continuum operators. The construction assures conservation of vorticity and mass and provides a determination of the local grid connectivity based on convergence criteria for the solution of Poisson's Equation. Extensions of the model have been made in the same spirit: finite-difference operators conform to the continuum limit and physical quantities are conserved properly. An important factor to note is that development of this method is entirely original work; there is no basic lore to fall back on when something goes wrong, and algorithms for a particular type of term must be devised and the best one chosen.

To date the basic hydrodynamic code incorporates algorithms which allow us to include the effects of surface tension and viscosity. These algorithms have been incorporated and tested extensively as described below. We have also devised algorithms for including the effects of compressibility for subsonic flow and for incorporating the effects of thermal conductivity. While these latter effects are being tested and incorporated, we will be developing the algorithms for vaporization and molecular diffusion. The final steps will allow us to describe a burning droplet.

The test problems performed have included simulations of incompressible flows about droplets in which the density ratios of droplet to background material have been 2:1, 10:1, and most recently 800:1. The two lower density ratios were used to test the various algorithms. The latest tests are aimed at modeling kerosene in air and have incorporated the expressions for surface tension and viscosity.

As an example of the way in which development of algorithms has proceeded, we describe the latest development in an algorithm for viscosity. Our viscosity algorithm originally expressed the change in the vorticity,  $\xi$ , at a grid point

due to viscosity by  $d\xi/dt = \nu \nabla^2 \xi$ , where  $\nu$  is the viscosity coefficient. All triangle velocities about a vertex contributed equally to the change in vorticity at the central grid point. Although the algorithm produced the correct spreading rates for the test case of a shear profile, we found that it only did so for fairly regular grid geometries because of the ambiguity in determining how the changes in vorticity are translated to velocity changes for different grid geometries. For an arbitrary grid, a more complete prescription was necessary and a method was developed in which  $\nabla^2 \bar{v}$  is a triangle-centered quantity.

This new triangle-centered algorithm was tested in a calculation of the spreading of a shear layer of initially zero thickness. The way in which the velocity distribution across this layer evolves and the growth of the width of the layer are known quantities which may be compared to the results of calculations. We found that the calculated layer width agreed exactly with the theory and the shear layer velocities were correct over the entire mesh. The components of velocity perpendicular to the shear layer remained zero indicating that the algorithm worked well even for the distorted grid used in the test problems.

In order to test our algorithm for surface tension, we performed calculations of droplets which oscillate under the effects of surface tension. The results of simulations could be compared to the linear theory for small amplitude oscillations on cylindrical jets, as first given by Rayleigh. We extended this theory to predict droplet oscillation frequencies for a droplet in a background gas of finite density.

In the numerical calculations we studied an  $n = 2$  oscillation for a droplet density of  $2 \text{ g/cm}^3$  and an external fluid density of  $1 \text{ g/cm}^3$ . From the calculations shown in Figure 1, we find that the numerical oscillation period is approximately  $1.25 \times 10^{-3} \text{ s}$  whereas the theoretical period is  $1.13 \times 10^{-3} \text{ s}$ . Most of the small discrepancy between the numerical and theoretical results can be explained by the finite grid spacing. However, given Rayleigh's experience with large amplitude oscillations, it is reasonable to expect our computational period to differ somewhat from that given by the linear theory.

Figures 2 and 3 show other early test calculations. Figure 2 illustrates the case for which the density ratio is 2:1 and there is no surface tension or viscosity present. We see that a recirculation zone forms early in the calculation, compressing the droplet in the direction parallel to the flow. Flow within the droplet is initiated by this compression in a direction normal to the external flow. The bulges formed at the top and bottom of the distorted droplet are pulled around the recirculation zone by the shear flow which is at a maximum at these points. The internal droplet flow is therefore driven by the compression set up between the front and rear stagnation points and by the high shear flow which extends around the top and bottom of the droplet and recirculation zone. The interaction of the droplet back onto the external flow occurs primarily through the enlarged cross-sectional area of the droplet which increases the size of the recirculation zone. Eventually the droplet is squeezed into a thin layer coating the recirculating zone. The thinned film then shatters into several smaller pieces, first at the rear of the droplet and later in the more laminar flow toward the front on the droplet.

Figure 3 shows the results of a calculation with surface tension for the same initial conditions as used in the calculation without surface tension (Figure 2). As in the case without surface tension, the internal droplet flow is driven by compression parallel to the external flow and is initially normal to the external flow. A recirculation zone is formed in the wake of the compressed droplet and the droplet is deformed as it is swept outward and backward by the external flow both outside and inside the recirculation zone. However, the presence of surface tension provides counteracting forces at regions of high curvature. Such forces at the sides and rear of the droplet are sufficient to stop the droplet from thinning around the recirculation zone.

The presentation will summarize the calculations shown above and then proceed to describe the more recent calculations at an 800:1 density ratio. Introducing this large ratio initially caused several problems in defining velocities when cells near the droplet boundary were divided. This problem was due to finite resolution effects at the boundary and has been fixed. Current simulations with viscosity should give us a realistic picture of flows in the droplet itself.

Finally, we describe the new algorithms to be tested for subsonic compressibility and thermal conductivity. A new parametric representation of taut splines will also be presented. This extension was necessary to achieve a "wiggle-free" spline fit in smooth regions of a droplet interface which were near surface discontinuities.

#### References

1. M.J. Fritts and J.P. Boris, "The Lagrangian Solution of Transient Problems in Hydrodynamics using a Triangular Mesh," J. Comp. Phys. 31, 173 (1979).
2. M.J. Fritts, D. E. Fyfe, and E.S. Oran, "Numerical Simulation of Droplet Flows with Surface Tension," Proceedings of the ASME Annual Winter Meeting, November 14-19, 1982.

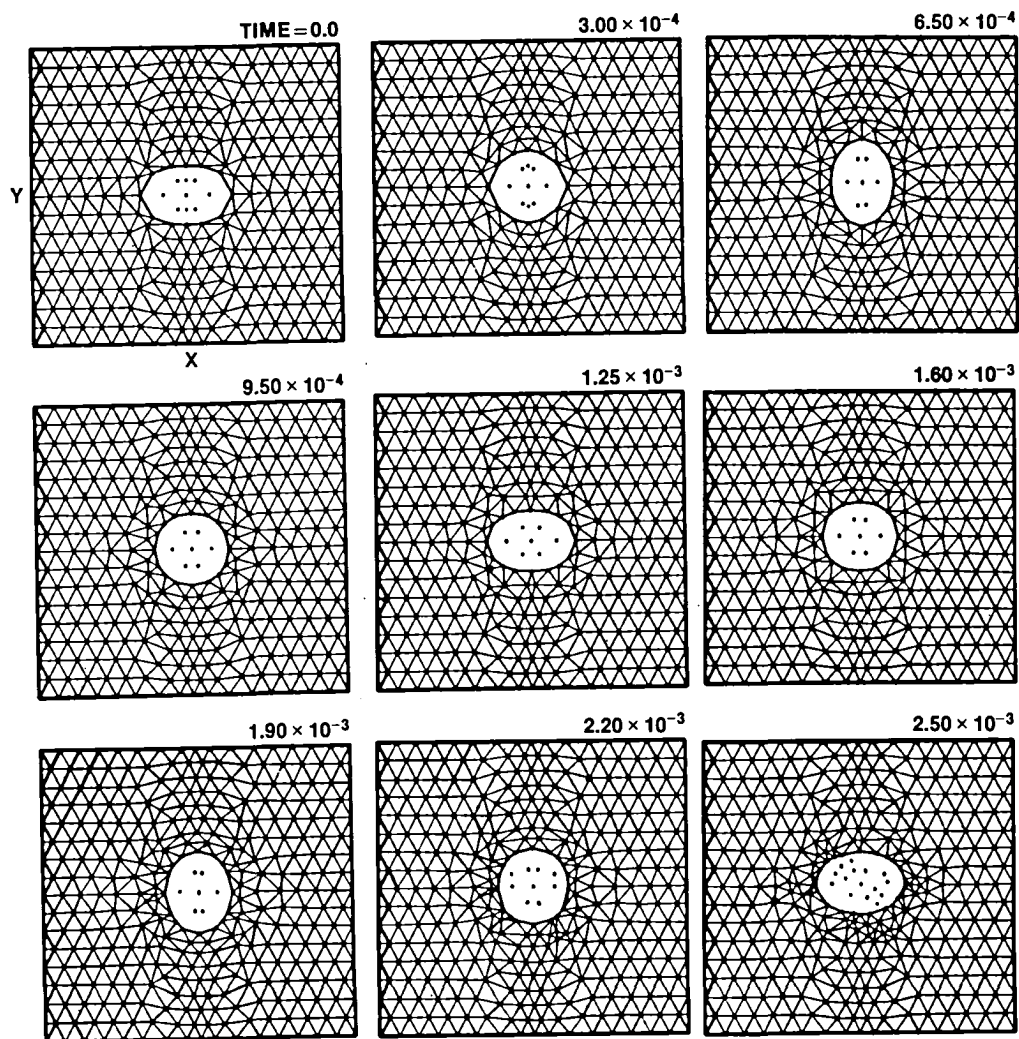


Figure 1

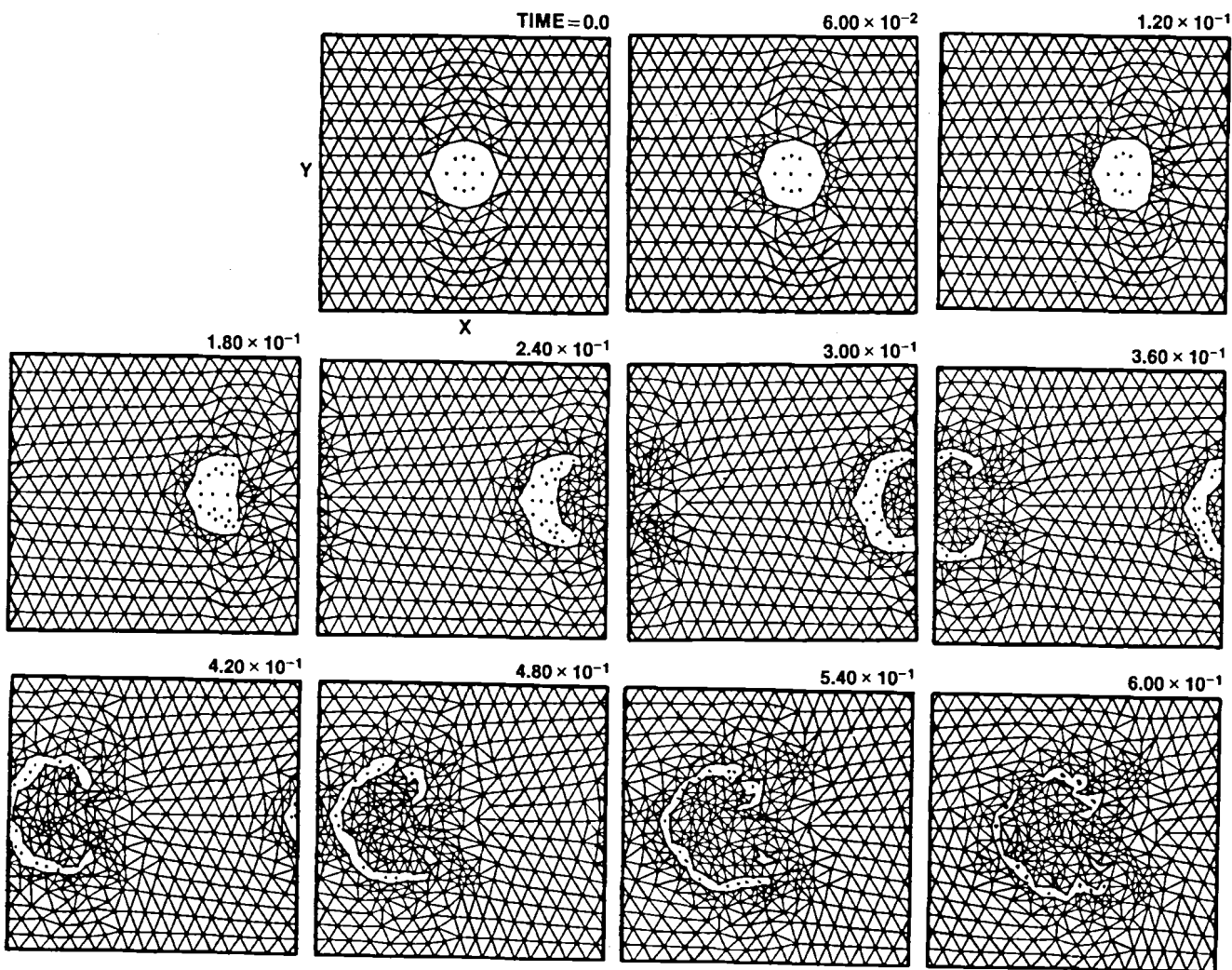


Figure 2

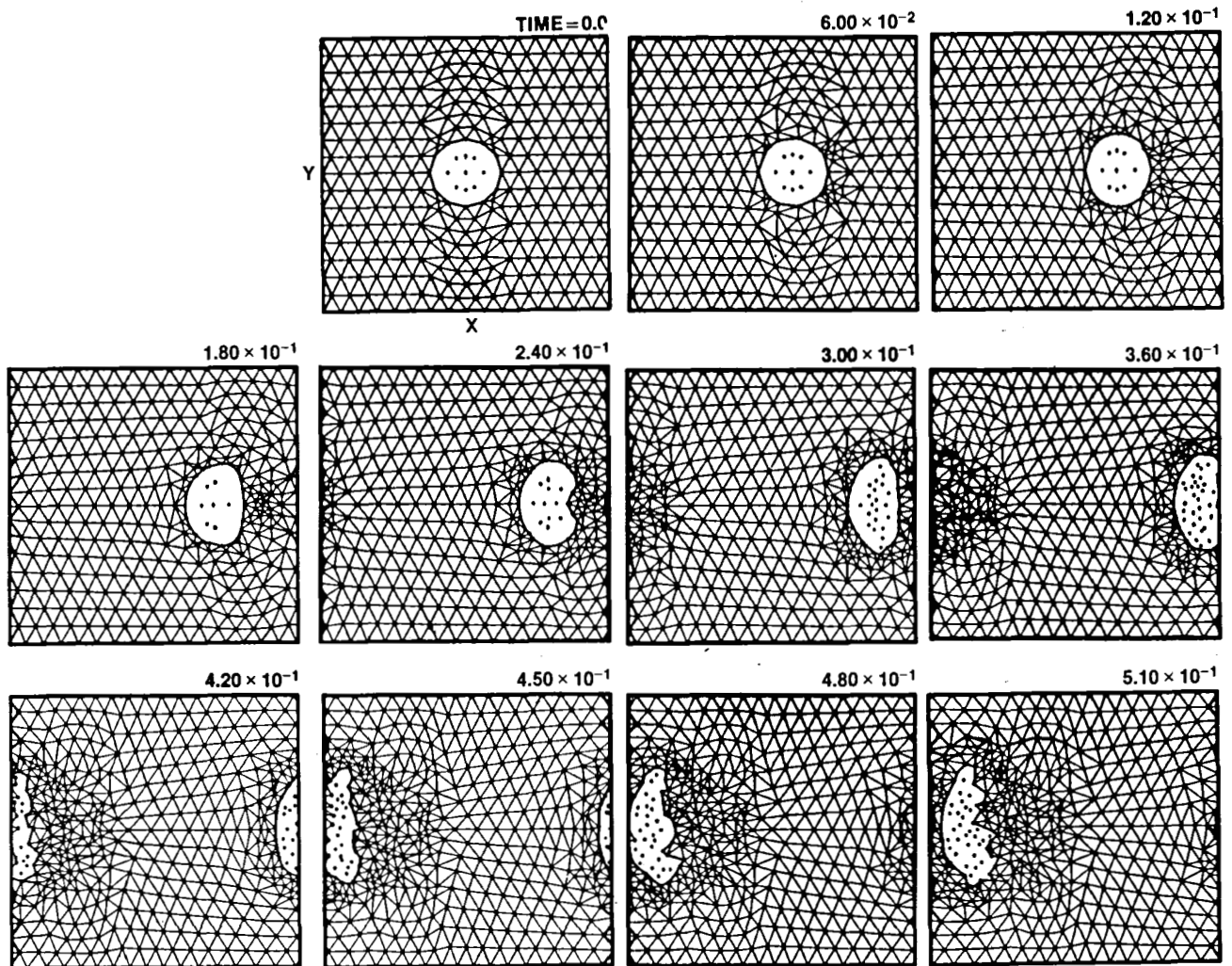


Figure 3